REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-00-

0400

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DAT...	3. ... COVERED
		1 April 1997 - 31 December 1999

4. TITLE AND SUBTITLE
Application of Control Theory and Design to Atomnic Scale Problems

5. FUNDING NUMBERS
F49620-97-1-0168

6. AUTHOR(S)
Mohammed Dahleh

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of California
Deparment of Mechanical Engineering
Santa Barbara, CA 93106

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR
801 N. Randolph Street, Room 732
Arlington, VA 22203-1977

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
F49620-97-1-0168

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION AVAILABILITY STATEMENT
Approved for Public Release.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*
The research program investigated two aspects of interactions between control theory and atomic scale sensing and modification of materials. One research focus was on a class of nanoscale sensors and actuators that are based on a microcantilever mechanism. The other direction was concerned with laser molecular control.

14. SUBJECT TERMS

15. NUMBER OF PAGES
14

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT

Application of Control Theory and Design to Atomic Scale Problems

Grant Number AFOSR: F49620-97-1-0168

Mohammed Dahleh
Department of Mechanical Engineering
University of California
Santa Barbara, CA, 93106.

Tel: 805-893-2704
Fax: 805-893-8651
e-mail: dahleh@engineering.ucsb.edu

Final Report

Contents

1 Objectives

Control theory is currently making an impact on the design of nanoscale sensors and actuators, and on the development of tools for material manipulation and identification at the molecular scale. The capability of using lasers to affect chemical reactions by direct manipulation, or indirectly by providing the means to unravel the underlying dynamical structure, is opening up the possibility for many applications. In addition, newly developed imaging and manufacturing tools are capable of resolving and altering atomic level features through mechanical interactions.

The objectives of this research program are to investigate two aspects of this interaction between control theory and atomic scale sensing and modification of materials:

- One direction of this research is focused on a class of nanoscale sensors and actuators that are based on a microcantilever mechanism. This is a wide class of important systems that include atomic force microscopes and nanoscale cutting tools. A complete analysis of the dynamics and control of such microcantilever structures is very important for their design and operation. The objective is to study the dynamical nature of microcantilevers interacting with surface forces under open and closed-loop operations. The results of this research are intended to provide the guidelines for the hardware design of microcantilevers and their control.

- The second direction is concerned with laser molecular control. The objective is to study the dynamical structure of controlled molecular systems, achievability of molecular objectives, and the identification of molecular potential energy surfaces using *pump-probe* experiments via system theoretic identification techniques.

2 Accomplishments and New Findings

2.1 Analysis and Control of Microcantilevers in Atomic Force Microscopy

A typical Atomic Force Microscope (AFM) consists of a microcantilever with a small tip, a piezo sample positioner. a detection system and a control system. The sample is scanned by moving the microcantilever over the sample in a rastering fashion. When the sample is close enough to the microcantilever, it exerts a large enough force to deflect the microcantilever. A laser incident on the top surface of the microcantilever

is reflected into a photodiode array and is used to detect the motion of the microcantilever. The control system regulates the position of the sample based on the photodiode output by adjusting the deflection of the piezo positioner. The piezo voltage, which is proportional to the tip-surface force interaction, provides a force image of the sample. A schematic representation of the atomic force microscope is shown in Figure 1.

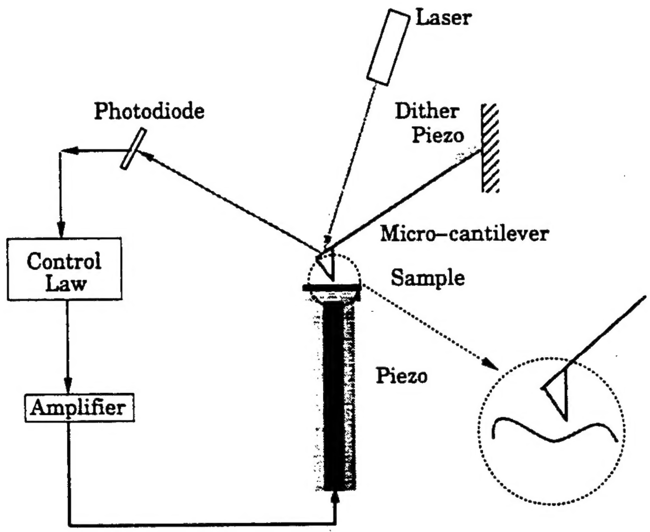

Figure 1: Schematic representation of the atomic force microscope setup.

2.1.1 Experimental Setup

We completed the installation of a Multimode (AFM), manufactured by Digital Instruments, in our laboratory. A vibration isolation system was constructed to reduce building vibrations. A digital signal processing (DSP) card with a Texas Instrument's chip provides the computational power for control implementation. The interface between the DSP card and the Pentium processor has been completed, which uses the dual port memory available on the DSP board and provides fast data transfer from the card to the pentium host. The data from the card is accessible to Matlab for further processing. The user interface that we built allows for downloading of code onto the DSP card, which makes it easy to implement control algorithms.

We completed a major redesign of the AFM by constructing optical sensors for the lateral movement of the piezo positioner with 10 nm resolution. System identification of the transfer function of the piezo

tube for x-y-z motions was completed [3, 24]. A feedback control system that can position the AFM tip on a sample with 10 nm resolution was constructed. This AFM is now used for conducting experiments for the identification and dynamical analysis of microcantilevers, the analysis of surface-cantilever interactions, and for carrying out nano-scale cutting experiments. We applied the newly developed positioning system to conduct imaging experiments of biological cells in collaboration with the Neurosciences Research Institute at UCSB. The selective positioning system that we developed is crucial to tracking different features in neuronal cells.

2.1.2 Microcantilever-sample Dynamics and Control

In one of the most popular modes of imaging, the *tapping mode*, the cantilever is vibrated near its resonant frequency by a dither piezo (see Figure 1). The behavior of the cantilever under such a forcing depends on the sample surface and material characteristics. By monitoring the vibration of the cantilever, information on the sample is obtained. The cantilever-sample interaction is nonlinear, and standard techniques of using a linear model fail to describe the behavior of the cantilever in the *tapping mode* operation.

We modeled the microcantilever as a single spring-mass-damper system, and the microcantilever-sample interaction via a Lennard-Jones potential which describes the experimentally observed features of long range attractive forces and short range repulsive forces. Based on this model, we studied the behavior of the cantilever under a sinusoidal forcing. In particular, the phase portrait of the dynamics was obtained for a range of the cantilever-sample distances. We showed that in a relevant range of operation, the phase portrait consists of two homoclinic orbits filled with periodic orbits. Using Melnikov method, we analyzed the dynamics of the microcantilever sample system when the microcantilever is subjected to a sinusoidal forcing. We determined the region in the space of physical parameters where chaotic motion is present [1, 14]. Using a proportional and derivative controller we computed the Melnikov function in terms of the parameters of the controller, and showed how the controller parameters can be designed to selectively change the regime of dynamical interaction [15].

Using nonlinear analysis techniques on attracting limit sets, we numerically verified the presence of chaotic invariant sets. The chaotic behavior appears to be generated via a cascade of period doubling, whose occurrence has been studied as a function of the system parameters [18]. We experimentally observed period doubling bifurcations at our AFM laboratory at UCSB [9]. As expected, the chaotic attractors are

obtained for values of parameters predicted by Melnikov theory. In addition to explaining the experimentally observed chaotic behavior, this analysis can be useful in finding a controller that stabilizes the system on a non-chaotic trajectory. The analysis can also be used to change the AFM operating conditions to a region of the parameter space where regular motion is ensured [18].

2.1.3 Stability and Sensitivity of Periodic Orbits in Tapping Mode AFM

After developing a nonlinear dynamical model for a forced microcantilever-sample system, we showed that the system exhibits periodic motion with period equal to that of the forcing. Using the Poincare map technique we established the orbital stability of the periodic motion, and obtained the sensitivity of the Poincare map's fixed point with respect to the microcantilever-sample distance. The sensitivity study of the fixed point has shown that the amplitude and sine of the phase of the orbit vary linearly with respect to the microcantilever-sample distance. Experiments conducted on a silicon microcantilever agree with the theory developed. These results will make it possible to probe and image the elastic properties of a sample by providing a measurement of the sample's coefficient of restitution [22].

2.1.4 Modeling and Control of Multicantilever Arrays

Throughput in atomic force microscopes is limited by the mechanical properties of the microcantilevers and by the detection and control design. A very important objective is to increase the throughput by improving both the design of the microcantilevers and the control system. Recently a new approach for increasing the throughput was developed where an array of microcantilevers are used to simultaneously image a surface. Control of the individual microcantilevers is achieved by a piezoelectric actuator and a piezoresistive sensor integrated on the microcantilever.

In this work we derived a model for an array of microcantilevers that are connected to each other through a common base, and are individually actuated. The sensors are also integrated on each microcantilever. This system is an example of a spatially-invariant system with a *distributed array of sensors and actuators.* We exploited the spatial invariance of the problem to design optimal $\mathcal{H}_2$ controllers for this array. We derived an analytic expression for the optimal controller in the transformed domain, and estimates of the communication range of each controller with neighboring microcantilevers [8].

2.1.5 Repeated Impact Oscillators and Stochastic Resonance

We studied a model for repeated impacts of a mass attached to a spring with a massive, sinusoidally vibrating table. This model represents the cantilever-sample dynamics in atomic force microscopy. In this work, we have shown that for some values of the frequency of the vibrating table, there are countably many orbits of arbitrarily long periods and the system is sensitive to initial conditions. The results are in agreement with experiments that we previously conducted on our atomic force microscope.

Stochastic resonance (SR) is an interesting phenomenon which can occur in bistable systems subject to both periodic and random forcing. This effect produces an improvement of the output signal-to-noise ratio when the input noise increases. In this research we derived an expression for the power spectral density of a general class of systems revealing SR phenomena. This result will have several useful applications in many technological contexts such as the analysis of the effects of thermal noise in Atomic Force Microscopy, in order to optimize the achievable resolution for imaging.

2.2 Mixed Objective Robust Control Design

In [5] we developed a complete solution for the MIMO mixed objective control synthesis problem, where the $\mathcal{H}_2$ norm is minimized subject to ℓ_1 constraints. The solution is efficient and reduces to solving a quadratic programming problem. In addition to its fundamental value in the theory of feedback, the importance of this methodology is that it enables the control design engineer to add several performance and robustness objectives with a modest increase in the computational complexity of the problem. In [16], a new approach based on generating convergent upper and lower bound approximations was developed. The novelty of this method is that it does not involve the use of zero interpolations which significantly simplifies the solution of the approximation problems.

In the presence of system uncertainties, a controller must be designed that delivers good performance in the presence of the worst case perturbation. The problem of synthesizing a controller to achieve robust performance is very difficult and requires the solution of a nonconvex problem. There are very few scenarios that can lead to computable results. Recently, we solved the problem of control synthesis for nominal $\mathcal{H}_2$ and robust ℓ_1 performance with scalar perturbations [21].

2.3 Quantification and Control of Fluid Mixing

We initiated a research direction, that aims at quantifying and controlling fluid mixing processes. We showed that the Kolmogorov-Sinai entropy provides a good measure for both the quality and speed of mixing. A *prototypical* fluid flow process, which is typically used to model mixing, is composed of horizontal and vertical shears. This process describes the basic stretching and folding mechanisms involved in mechanical mixing. In [2, 17] we solved the optimal control problem of choosing the sequence of horizontal and vertical shears that maximizes entropy. The development of these results required the extension of several tools from ergodic theory that apply to a single transformation to the case of *sequences* of transformations [10, 20].

2.4 Control of Quantum Systems

2.4.1 Optimal Control of Two-level Quantum Systems

This research is motivated by the design of quantum mechanical logic gates which perform prescribed logic operations on a two-level quantum system, a *quantum bit.* The problem that we solved is that of driving the evolution operator of the system to a desired state, while minimizing an energy-type cost. Mathematically, this problem translates into an optimal control problem for systems varying on the Lie group of special unitary matrices, with a quadratic cost on the control. In the process we developed a comprehensive theory of optimal control for two-level quantum systems. In particular, we proved the 'normality' of the given problem and the 'regularity' of the optimal control functions. The results of this research will have an impact on nuclear magnetic resonance experiments and quantum computation.

2.4.2 Controllability in Two-Spins Magnetic Resonance Experiments

We considered a system of two interacting spin $\frac{1}{2}$ particles in a magnetic field. The magnetic field is assumed to have a constant component in a given spatial direction and an orthogonal component which may vary with time. Under the standard assumption of different gyromagnetic ratios for the two spins, we provided a rigorous proof of the following important fact: It is possible to obtain every spin configuration by appropriately varying the magnetic field as a function of time. The proof utilizes several results on controllability of systems on Lie groups.

3 Transitions and Interactions

The objectives pursued under this program are of great interest to industry and to DOD research that involves microscopy and micro/nano-manufacturing. Research findings are systematically relayed to the engineering community through the participation in conferences (e.g. ACC, CDC and ASME), and the organization of special sessions and workshops. A close cooperation with industry, in particular with Digital Instruments, Ford, SurForce, and Raytheon is in place.

In addition to the fundamental work that we are pursuing under this program, we are developing a system for accurate selective positioning of piezo tubes with nano-scale resolution. This system will allow the user to conduct a large scan and then selectively focus on a portion of the scan for more accurate imaging. This novel system, which involves hardware design (optical lever sensors), identification, control, and image processing will soon be available. We expect such a system to have applications that go beyond microscopy.

The following are specific interactions:

Performer: M. V. Salapaka
Customer: Digital Instruments, Santa Barbara
Contact: Dr. Jason Cleveland, jc@di.com
Result: M. V. Salapaka spent 8 weeks at Digital Instruments where he developed a method for the characterization of surface elastic properties based on tapping mode atomic force microscopy. The slope of the curve of the amplitude of vibration of the cantilever vs. tip-surface separation, as well as the slope of the sine of the phase vs. tip-surface separation, provide formulas for the determination of the coefficient of restitution of the surface. Such measurements were not possible before this analysis.
Application: Functions to measure and display the curves of amplitude and phase vs. tip-surface separation can be added to the new generation of atomic force microscopes for high resolution imaging. Using these functions the mechanical properties of surfaces can be imaged.

Performer: A. Daniele, M. V. Salapaka
Customer: Digital Instruments, Santa Barbara
Contact: Dr. Jason Cleveland, jc@di.com

Result: Tutorial lectures on feedback control for piezo positioning presented at UCSB to members of the technical staff of Digital Instruments.
Application: The techniques are to be used in the design of control systems for z-axis control of commercial atomic force microscopes.

Performer: M. Dahleh, N. Karlsson
Customer: Ford Motor Company
Contact: D. Hrovat, dhrovat@ford.com
Result: A new nonlinear control design methodology that optimizes quadratic and quartic cost functions.
Application: The technique was applied to the design of active control of suspension systems with and without preview. The methodology is being developed to address other automotive applications.

Performer: M. Dahleh
Customer: Control Community
Contact: M. Dahleh, dahleh@engineering.ucsb.edu
Result: Organized the Workshop "Dynamics, Control and Computation", April 2-3, 1998, Santa Barbara. Attendees included faculty, students and members of industry.
Application: The lectures presented several applications and methods that are developed under this program.

Performer: M. Dahleh, A. Vicino, A. Tesi, and G. Zappa
Customer: Control Community
Contact: A. Vicino, vicino@unisi.it
Result: Organized the Workshop "Robustness in Identification and Control", July 30 - August 2, 1998, Siena, Italy.
Application: The lectures presented several applications and methods that are developed under this program.

Performer: M. Dahleh, N. Karlsson, Department of Mechanical Engineering, University of California, Santa Barbara, CA 93106. Phone: 805-893-2704.
Customer: Ford Motor Company, P.O. Box 2053, Dearborn, MI 48121-2053, Phone: 313 322 1492.
Contact: D. Hrovat, Phone: 313 322 1492, dhrovat@ford.com.
Result: Multi-objective control design to meet time-domain and frequency-domain criteria.

Application: The techniques on multi-objective control design that were developed under this program are applied to the design of active control of suspension systems with and without preview. Comparisons are made with nonlinear controllers that optimize a quartic performance index.

Performer: M. Dahleh, Department of Mechanical Engineering, University of California, Santa Barbara, CA 93106. Phone: 805-893-2704.

Customer: SurForce Corporation, 5385 Hollister Ave # 313, Santa Barbara, CA 93111. Phone: 805-692-1690.

Contact: G. Gasga, Phone: 805-692-1690.

Result: Sensing and control methods for atomic force microscope scanners.

Application: The sensing, control and imaging methods that were developed under this program are used to build a new atomic force microscope scanner. The scanner is based on an arrangement of piezo-electric parts with a high positioning sensitivity.

4 Personnel Supported

Principal Investigator

- Mohammed Dahleh

Graduate Students

- Andrew Daniele.
- Sami Ashhab.
- Domenico D'Alessandro.

5 Honors/Awards

Elected Fellow of IEEE, 1999.

6 Publications

1. M. Ashhab, M. Salapaka, M. Dahleh, and I. Mezic, "Control of Chaos in Atomic Force Microscopes," *Proceedings of the American Control Conference*, Albuquerque, New Mexico, pp. 196-202, June, 1997.

2. Domenico D'Alessandro, M. Dahleh, and I. Mezic, "Maximum Entropy Approach to the Control of Mixing," *Proceedings of the American Control Conference*, Albuquerque, New Mexico, pp. 160-161, June, 1997.

3. A. Daniele, T. Nakata, L. Giarré, M. V. Salapaka and M. Dahleh, "Robust Identification and Control of Scanning Probe Microscope Scanner," *Proceedings of the 2nd IFAC Symposium on Robust Control Design, 1997*, pp. 37-42.

4. S. Salapaka, M. Dahleh, and L. Giarre, "Filtering of Nonlinear Chaotic Time-Series with Noise" *Proceedings of the 36th Conference on Decision and Control*, San Diego, CA, pp. 1669-1771, December, 1997.

5. M. Salapaka, M. Dahleh, and P. Voulgaris, "Mixed Objective Control Synthesis: Optimal $\ell_1/\mathcal{H}_2$ Control," *SIAM Journal on Control and Optimization,* Vol. 35, No. 5, pp. 1672-1689, 1997.

6. B. Bamieh, and M. Dahleh, "On Robust Performance in $\mathcal{H}^\infty$", *Systems and Control Letters*, Vol. 33, pp. 301-305, 1998.

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8. M. Napoli, B. Bamieh, and M. Dahleh, "Optimal Control of Arrays of Microcantilevers," *Proceedings of the Conference on Decision and Control*, Tampa, Florida, pp. 2077-2082, December 1998.

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11. A. Daniele, S. Salapaka, M. V. Salapaka, and M. Dahleh, "Piezoelectric Scanners for Atomic Force Microscopes: Design of Lateral Sensors, Identification and Control, " *Proceedings of the American Control Conference*, San Diego, CA, pp. 253-257, June 1999.

12. B. Bamieh and M. Dahleh, "Disturbance Energy Amplification in Three-Dimensional Channel Flows," *Proceedings of the American Control Conference*, San Diego, CA, pp. 4532-4537, June 1999.

13. M. Basso, M. Dahleh, I. Mezic, and M. V. Salapaka, "Stochastic Resonance in AFMS, " *Proceedings of the American Control Conference*, San Diego, CA, pp. 3774-3778, June 1999.

14. M. Ashhab, M. V. Salapaka, M. Dahleh, and I. Mezic, "Dynamical Analysis and Control of Microcantilevers," *Automatica*, Vol. 35, No. 10, pp. 1663-1670, October 1999.

15. M. Ashhab, M. V. Salapaka, M. Dahleh, and I. Mezic, "Melnikov-based Dynamical Analysis of Microcantilevers in Scanning Probe Microscopy," *Journal of Nonlinear Dynamics,* Vol. 20, pp. 197-220, 1999.

16. M. V. Salapaka, M. Khammash, and M. Dahleh, "Solution of MIMO $\mathcal{H}_2/\ell_1$ Problem without Zero Interpolation," *SIAM Journal on Control and Optimization,* Vol. 37, No. 6, pp. 1865-1873, 1999.

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18. M. Basso, L. Giarre', M. Dahleh, "Complex Dynamics in a Harmonically Excited Lennard-Jones Oscillator: Microcantilever-Sample Interaction in Scanning Probe Microscopes, " *accepted in ASME Journal of Dynamic Systems Measurement and Control.*

19. B. Bamieh and M. Dahleh, "Energy Amplification in Channel Flows with Stochastic Excitation," *accepted in Physics of Fluids.*

Submitted

20. D. D'Alessandro, I. Mezic, and M. Dahleh, "Some Ergodic Theorems for Sequences of Measure Preserving Transformations ," *submitted to the Journal of Statistical Physics.*

21. M. V. Salapaka, M. Dahleh, A. Tesi, and A. Vicino, "Nominal $\mathcal{H}_2$ Performance and ℓ_1 Robust Performance," *submitted to IEEE Trans. Automat. Contr.*

22. M. V. Salapaka, D. J. Chen, and J. P. Cleveland, "Stability and Sensitivity Analysis of Periodic Orbits in Tapping Mode Atomic Force Microscopy," *submitted to Physical Review B.*

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23. B. Bamieh and M. Dahleh, "Analysis of Stochastically Perturbed Channel Flow," CCEC Report SB 98-8-17.

24. A. Daniele, S. Salapaka, M. V. Salapaka, and M. Dahleh, "Design of Lateral Motion Sensors, Identification and Control of Piezo-Sensor System in Atomic Force Microscopes," CCEC Report SB 98-8-27.

Theses

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26. M. Ashhab, "Dynamical Analysis and Application of Advanced Control Techniques to Atomic Force Microscopes and Camless Engines", UCSB, June 1998.

27. A. Afifi, "Dynamical Analysis of Scanning Force Microscopy Using Matlab," Masters Thesis, UCSB, December 1998.

28. D. D'Alessandro, "Ergodic Theory and the Control of Mixing in Fluid Flows, " PhD Thesis, May 1999.